Regularization of Particle Transport Models with Diffusive Relaxation

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We present recent progress on numerical methods for a family of linear hyperbolic balance laws with stiff diffusive relaxation that model particle transport in a material medium. In diffusive regimes, conventional hyperbolic solvers for these systems suffer from excessive numerical dissipation, numerical stiffness, or both. We have developed a regularization technique to address such issues at the continuum level.

In kinetic models of particle transport, diffusive relaxation is a common phenomenon that occurs when the mean free path between particle collisions with a material medium is small when compared with the macroscopic scales of interest. In such cases, particles undergo frequent collisions with the material so that, over long time scales, the predominant macroscopic behavior of the system is diffusive.

We are specifically interested in simulating the time-dependent P_N equations, a linear hyperbolic system of $N + 1$ moment equations that is used to approximate kinetic transport in neutron and photon applications. Using operator-splitting techniques, we have formally derived a regularized version of the P_N system for which the diffusive limit is explicitly built-in. Our method is a nontrivial extension of an approach used in [1]. It applies to a large family of balance laws, allows for large time steps, and handles spatial variations in the material medium, which affect the local collision rate. Moreover, the regularization does not suffer from oscillations that sometimes appear in other splitting methods [4].

The derivation of the regularized P_N system proceeds in three steps: 1) separation of the equations into two subsystems, each containing either fast or slow dynamics; 2) discretization of each subsystem in time, keeping spatial derivatives in continuum form; and 3) recombining the semidiscretized subsystems and taking specific limits to get back the continuum time derivative. The result is a hyperbolic-parabolic system with the following properties [2,3]:

- In diffusive regimes, standard numerical methods for the regularized equations capture the diffusion limit with a mesh spacing based on the macroscopic solution profile and not the mean free path. This is the so-called asymptotic preserving (or AP) property [1].
- In cases where the mean free path is not resolved by the spatial mesh, there is no hyperbolic Courant-Friedrichs-Lewy (CFL) condition. Thus an implicit discretization of the diffusion operator allows for large time steps. Moreover, the diffusion operator is diagonal, so that implicit solvers are relatively easy to implement.
- In streaming regimes, where the mean free path is relatively large and collision rates are low, the regularized system behaves like the standard P_N equations.

Computational results for 1D test problems confirm that the regularization gives accurate results in different regimes and that, in the diffusion regime, it does so at a fraction of the cost of upwind or discontinuous Galerkin solvers for the original P_N system.

Results from a sample simulation are given in Figs. 1 and 2, where the particle concentration based on a P3 calculation is plotted. An important parameter here is the cell optical depth, which gives the number of mean free paths in a computational cell. When this value is large, upwind schemes tend to be overly dissipative and numerically stiff. These results confirm the properties of the regularization outlined above.

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[3] C.D. Hauck et al., LA-UR-08-04966 (2008) to appear in *Numerical Methods for Relaxation Systems and Balance Equations, Quaderni di Matematica*.
[4] J.R. Haack, C.D. Hauck, LA-UR-08-0571 (2008) *Kinet. Related Model* **1,** 573-590.

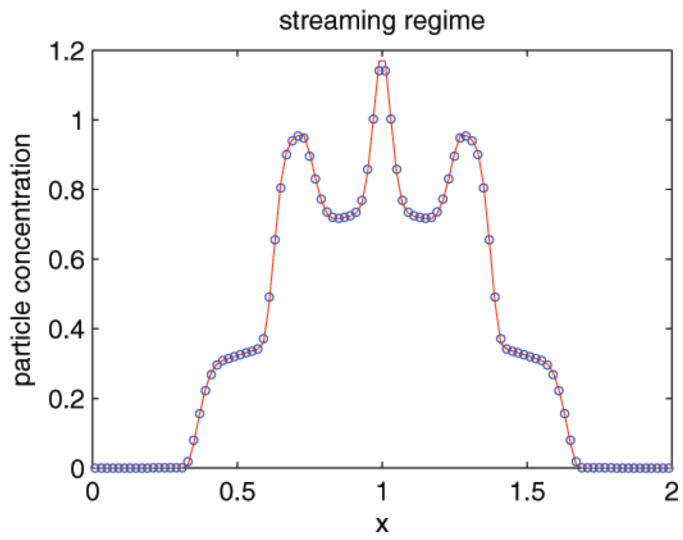

Fig. 1. Snapshot in time of the particle concentration for P3 (red line) and regularized P3 (blue circles). The initial condition is a characteristic function with height two and support [0.8,1.2]. Both computations use upwind methods that are first order in time and second order in space, with 100 spatial cells and a CFL number of 0.1. The cell optical depth is 0.01.

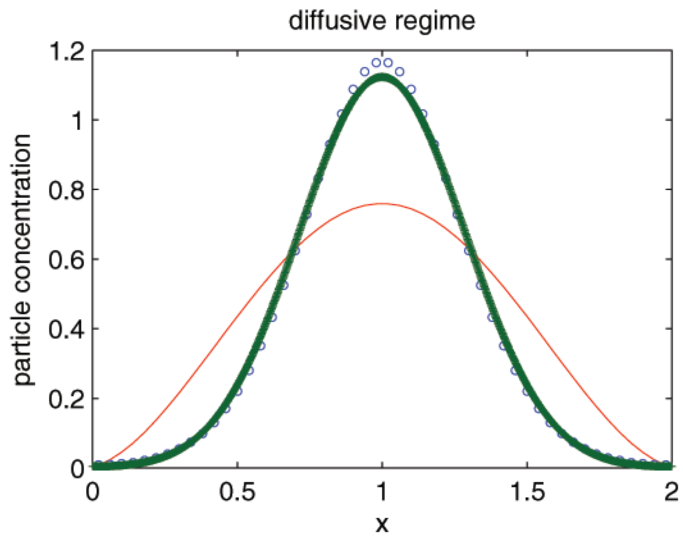

Fig. 2. Repeat of Fig. 1, but with 50 spatial cells and a cell optical depth of 250. Based on the CFL restriction, the P3 computation (red line) takes roughly 30,000 time steps, while the regularized version (blue circles) uses less than 10. The thick green line is a highly resolved numerical solution for the limiting diffusion equation.

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